INFRARED SPECTROSCOPY OF LARGER BENZENE-$(H_2O)_n$ HYDROGEN-BONDED CLUSTERS: EVIDENCE OF CUBIC STRUCTURES

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One color R2PI-TOFMS, ultraviolet hole-burning, and RIDIRS have been used to assign and characterize the hydrogen-bonding topology of size-selected benzene-$(H_2O)_n$ clusters formed in a supersonic molecular beam. Hole-burning spectroscopy confirms the presence of conformers in the increasingly congested R2PI spectra of these larger clusters. Two transitions in the benzene-$(H_2O)_6^+$ R2PI-TOFMS are assigned to the benzene-$(H_2O)_8$ cluster. Comparison of the experimental RIDIR spectra to density functional theory calculations results in the assignment of these conformers to cubic octamers of S_4 and D_{2d} symmetry. The presence of benzene weakly distorts the cubic structures, breaking the degeneracy of several OH stretch vibrations and inducing intensity in otherwise forbidden infrared transitions. Four transitions in the benzene-$(H_2O)_7^+$ R2PI-TOFMS are tentatively assigned as two conformers each of the $(\text{benzene})_2$-$(H_2O)_8$ and the benzene-$(H_2O)_9$ clusters. The RIDIRS of these species share common features with those of the cubic benzene-$(H_2O)_8$ octamers; thus, a structure for the benzene-water nonamer built by adding one water molecule to a cubic octamer is tested against calculations.